ORIGINAL ARTICLE



# Synthesis, Characterization and Solvatochromic Studies Using the Solvent Polarity Parameter, ENT on 2-Chloro-3-Ethylamino-1,4-Naphthoquinone

Arulappan Durairaj<sup>1</sup> · Asir Obadiah<sup>1</sup> · Subramanian Ramanathan<sup>1</sup> · Princy Merlin Johnson<sup>2</sup> · Antony Paulraj Bella<sup>2</sup> · Samuel Vasanthkumar<sup>1</sup>

Received: 4 January 2017 / Accepted: 4 April 2017 © Springer Science+Business Media New York 2017

Abstract Quinones are molecules with varied biological activities and electronic properties which are used for important applications [1, 2]. Quinone with a heteroatom substituted, namely 2-chloro-3-ethylamino-1,4-naphthoquinone (N-CAN) was synthesized and characterized by various techniques such as H1-NMR, C13-NMR, Mass spectroscopy and FT-IR spectroscopy. In this study, the solvatochromic effects on the spectral properties of 2-chloro-3-ethylamino-1,4naphthoquinone have been investigated in different solvents taking into consideration, the solvent parameters like dielectric constant ( $\varepsilon$ ) and refractive index (n) of different solvent polarities. Using Lippert-Mataga, Bakshiev's, Kawski-Chamma-Viallet and Reichardt equations, the ground state  $(\mu_{\sigma})$  and excited state  $(\mu_{e})$  dipole moments were calculated. The angle between the excited state and ground state dipole moments were also calculated.

**Keywords** 2-chloro-3-ethylamino-1,4-naphthoquinone · Lippert-Mataga, Bakshiev's · Kawski-Chamma-Viallet, Reichardt equations · Dipole moments

**Electronic supplementary material** The online version of this article (doi:10.1007/s10895-017-2090-6) contains supplementary material, which is available to authorized users.

Samuel Vasanthkumar kumar2359@yahoo.com

- <sup>1</sup> Department of Chemistry, Karunya University, Coimbatore, Tamilnadu 641114, India
- <sup>2</sup> Department of Chemistry, Bishop Heber College, Trichirapalli, TN 620017, India

#### Introduction

Photophysical studies are an important tool to bring out new technology and develop new organic non-linear optical materials. Optical absorption and fluorescence spectroscopy techniques reveal the solute-solvent interactions, which can be studied using the frequency, shape and the intensity of the spectrum. Spectral shift results are due to the difference in solvent polarity, specific solute-solvent interactions such as hydrogen bonding, acid base reactions and charge transfer interactions. Reorganisation of the solvent molecules around the newly formed excited solute molecules gives rise to the well-known stokes shifts. The magnitude of the spectral shifts depends strongly on the molecule excited and on the nature of the solvent. Generally, polar solvents give rise to larger shift [3]. The molecules are subjected to change in polarity on excitation and thus the solvent environment plays an effective role stabilizing or destabilizing the excited state, which may lead to a bathochromic (red, called positive solvatochromism) shift or a hypsochromic (blue, called negative solvatochromism) shift in the fluorescence emission spectrum of the molecules [4, 5]. Excitation of a molecule by photon cause the redistribution of charges in the excited state leading to conformational changes. The dipole moment of an electronically excited state of a molecule is an important property that provides information on the electronic and geometrical structure of the molecule in short-lived states. Knowledge of the excited-state dipole moment of electronically excited molecules is quite useful in designing nonlinear optical materials [6]. The excited dipole moment is expected to increase or decrease than the dipole moment of the ground state. The determination of excited-state dipole moment is derived using various techniques e.g. electronic polarization of fluorescence [7], electric-dichroism [8], microwave conductivity [9] and stark splitting [10], but every technique has some limitation because they are considered to be equipment sensitive. Among the techniques available for the determination of the excited-state dipole moments, the most popular one is that, which is based on Lippert–Mataga equation [11, 12], Bakshiev's equation [13], Kawski-Chamma-Viallet's equation calculations [14, 15] and Reichardt equation [16]. In this methodology, absorption and fluorescence shifts follow bulk solvent polarity, described by dielectric constant ( $\varepsilon$ ) and refractive index ( $\eta$ ).

Several workers have made extensive experimental and theoretical studies on ground ( $\mu$ g) and excited state ( $\mu$ e) dipole moments using different techniques on a variety of organic fluorescent compounds like coumarins [17], indoles [18], purines [19], exalite dyes [20], quinazolines [21], acridines and phenazine [22], anthraquinone [23], fluorescein [24], flavone [25], phthalamide [26], boronic acid [27], and pyrimidine [28] etc.

The quinone derivatives have a variety of structural and electronic properties. The electron uptake capacity of a given moiety can be introduced by directly adding substituent to the quinone structure. The electron donating and accepting system may be useful in the organic non-linear optics, and other applications. In this present study, the dipole moment of the quinone compound is evaluated both in the excited singlet state and ground state. The donor ligand of an amine group and acceptor ligand of a ketone has a compound influence on solvents of various polarities. Therefore the electronic absorption and emission spectra of the N-alkyl amino naphthoquinone (N-CAN) will be interesting to study. The (N-CAN) compound was synthesized, characterized and the dipole moments of the ground state and excited singlet states evaluated by Lippert-Mataga equation, Bakshiev's equation, Kawski-Chamma-Viallet equation and Reichardt correlation equation. The angle between the excited and ground state dipole moments is also calculated.

### **Experimental**

# Materials

The chemicals such as dicholoronaphthoquinone, triethylamine, ethylamine were purchased from Sigma-Aldrich, and used without further purification. The solvents used in the study like Hexane, Acetonitrile (ACN), Chloroform (CHCl<sub>3</sub>), Dimethylformamide (DMF), Ethanol, Methanol, 1,4-Dioxne, Acetone, Dicholoromethane (DCM), Ethylacetate (EA), Isopropyl alcohol (IPA) were purchased from sigma Aldrich India (HPLC grade).

#### Synthesis of N-Alkylamino Compound (N-CAN)

The process to be followed for the preparation of the building block of basic quinone compound is as follows: Dicholoronaphthoquinone (DCNQ) was dissolved in ethanol and refluxed. The mixture was heated to gentle boiling condition and the ethyl amine was added in drops slowly through the condenser. To this mixture, a small amount of the base triethylamine was added. The refluxing was continued for two to four hours, and to ensure the completion of reaction, it was monitored by TLC. The hot reaction solution was treated with cold water to get a red colour solid. The crude product was separated by filtration, washed with water to remove excess base and starting material. The compound was purified using column chromatography on silica gel (60–120 mesh) using Hexane: Ethylacetate (4:1) eluent system.

#### **Characterization Techniques**

Steady-state absorption spectra at room temperature (298 K) were recorded by dual beam Jasco V- 550 spectrometer. The emission spectra were recorded by using flurolog-3 photoluminescence and data were analyzed by the related software. The FT-IR were recorded by IR prestige 21 Shimadzu instrument. The <sup>1</sup>H NMR and <sup>13</sup>C spectra were recorded with the help of 400 MHz Bruker NMR spectrometer using CDCl<sub>3</sub> as the solvent and chemical shift values were in internal standard. For Absorption and emission measurements, samples were taken in 1 cm × 1 cm Quartz cells. The concentration of solvents used for the spectroscopy studies was  $10^{-4}$  mol dm<sup>-3</sup> in all cases.

#### **Ground State and Excited Dipole Moment**

Different methods are available for calculating the excited dipole moment of organic compounds. The solvatochromic method is a method used for determining the ground state and excited state dipole moment. The N-CAN compound ground state and excited state dipole moment were calculated using Lippert-Mataga equation [11, 12], Bakshiev's equation [13] and Kawaski-Chamma-Viallet's equation [14, 15]. The three equations are given below.

Lippert-Mataga equation:

$$\overline{v_a} - \overline{v_f} = Z_1 F_1(\varepsilon, \eta) + C \tag{1}$$

Bakshiev's equation:

$$\overline{v_a} - \overline{v_f} = Z_2 F_2(\varepsilon, \eta) + C \tag{2}$$

Kawaski-Chamma-Viallet equation:

$$\frac{\overline{\nu}_a + \overline{\nu}_f}{2} = -Z_3 F_3(\varepsilon, \eta) + C \tag{3}$$

In these equations  $F_1(\varepsilon, \eta)$ ,  $F_2(\varepsilon, \eta)$ ,  $F_3(\varepsilon, \eta)$  are the corresponding Lippert's polarity function, Bakshiev's polarity function, Kawaski-Chamma-Viallet polarity

function respectively. These polarity functions are expressed by the following equations

$$F_1(\varepsilon,\eta) = \left[\frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{\eta^2 - 1}{2\eta^2 + 1}\right] \tag{4}$$

$$F_2(\varepsilon,\eta) = \left[\frac{\varepsilon-1}{2\varepsilon+1} - \frac{\eta^2 - 1}{2\eta^2 + 1}\right] \frac{(2\eta^2 + 1)}{(\eta^2 + 2)} \tag{5}$$

$$F_{3}(\varepsilon,\eta) = \left[\frac{\varepsilon-1}{2\varepsilon+1} - \frac{\eta^{2}-1}{2\eta^{2}+1}\right] \frac{(2\eta^{2}+1)}{(\eta^{2}+2)} + \frac{3}{2} \frac{(\eta^{4}-1)}{2(\eta^{2}+2)^{2}}$$
(6)

Where  $\overline{v}_a$  and  $\overline{v_f}$  are the absorption and emission wavelength in cm<sup>-1</sup>. The symbols  $\varepsilon$  and  $\eta$  corresponds to the dielectric constant and refractive index respectively. The ground

state and excited state dipole moment are also evaluated by means of the following equations.

$$\mu_g = \frac{Z_2 - Z_1}{2} \left[ \frac{hca^3}{2Z_1} \right]^{\frac{1}{2}}$$
(7)

$$\mu_e = \frac{Z_2 + Z_1}{2} \left[ \frac{hca^3}{2Z_1} \right]^{\frac{1}{2}}$$
(8)

$$\mu_e = \left[\frac{Z_2 + Z_3}{Z_3 - Z_2}\right] \mu_g \quad (\text{for } Z_3 > Z_2) \tag{9}$$

The Suppan equation [29] gives the Onsager cavity radius of the molecules. Where 'M' denotes molecular weight, ' $\delta$ ' denotes the density of the solute molecule and 'N' denotes Avagadro number. The Suppan equation is given below.

$$a = \left(\frac{3M}{4\pi\delta N}\right)^{\frac{1}{3}} \tag{10}$$



Fig. 1 The absorption spectra of the N-CAN compound with changing solvent polarity

Reichardt proposed the microscopic solvent polarity scale  $E_{T}^{N}$  to overcome the error in the estimation of Onsager cavity. The  $E_{T}^{N}$  also takes into account the intermolecular solute and solvent, hydrogen bond donor and acceptor interaction [16, 30–34].

$$\overline{v}_a - \overline{v}_f = 11307.6 \left(\frac{\Delta \mu}{\Delta \mu_b}\right)^2 \left(\frac{a_o}{a}\right)^3 E_T^N + \text{Constant}$$
(11)

Where  $\Delta \mu_b = 9D$ , the change in dipole moment,  $a_o = 6.2$  Å the Onsager cavity radius of Betaine dye respectively.  $\Delta \mu$  and 'a' are the change in dipole moment and Onsager cavity radius of the molecule were taken under study.

Generally the dipole moments  $\mu_g$  and  $\mu_e$  are not parallel to each other but are having a small angle  $\phi$  between them and the angle ( $\phi$ ) calculated by the equation given below [34]

$$\cos\varphi = \frac{1}{2\mu_e\mu_g} \left[ \left( \mu_g^2 + \mu_e^2 \right) - \frac{Z_2}{Z_3} \left( \mu_e^2 - \mu_g^2 \right) \right]$$
(12)

# **Result and Discussion**

### **Spectroscopical Analysis**

The N-CAN compound was synthesised and analysed by spectroscopical studies. Mp: 124-126 °C, FT-IR (KBr, cm<sup>-1</sup>): NH (3271.41 cm<sup>-1</sup>), C-N (1295.29 cm<sup>-1</sup>), C = O (1680.07 cm<sup>-1</sup>), C-Cl (720.49 cm<sup>-1</sup>); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  8.00 (m, 2H),  $\delta$  7.6 (dd, 2H),  $\delta$  6.02 (1H, s),  $\delta$  3.9 (2H, q),  $\delta$  1.39 (3H, t); <sup>13</sup>C (MHz, CDCl<sub>3</sub>):  $\delta$  180.3, 143.9, 134.7, 132.1, 129.5, 125.6, 39.7, 16.13; MS:EI (m/e): 235.21.

#### **Electronic Absorption Spectra**

The ultraviolet absorption spectra of (N-CAN) in various solvents ranging from non-polar solvents to polar protic solvents are presented in Fig. 1. Non-polar solvents like n-hexane, toluene, borderline aprotic solvents like EA, DCM, polar aprotic solvents like acetone, ACN and polar



Fig. 2 The emission spectra of the N-CAN compound with varying polarity of solvents



Fig. 3 HOMO and LUMO geometry of N-CAN

solvents like methanol, ethanol were used in this study. The absorption spectra obtained are characterized by one sharp band for which the maxima was in the range 272 nm to 284 nm. The solvent effect due to polarity was obtained as a red shift for the absorption in all the solvents. The detailed study of stokes shift values was carried out for all polarity changes due to solvent changes. The results of the study indicate that the spectrum of N-CAN in all the solvents used is characterized by two electronic transitions, namely  $n \to \pi^*$  and  $\pi \to \pi^*$ . The presence of a unique transition in this solvent series may be explained only by the overlapping of  $n \to \pi^*$  and  $\pi \to \pi^*$ bands which are very close in energy. As the polarity of the solvents increases the magnitude of absorbance values also increase. All these go to indicate that the excited state is stabilized more when compared to the ground state.

Fluorescence Spectroscopy

The fluorescence spectra for N-CAN in different organic solvents are shown in Fig. 2. Florescence band maxima are largely bathochromic shifted when the solvent polarity increases. This fact indicates a higher dipole moment in the excited state than the dipole moment of the ground state. Interestingly by some molecules have opposite behaviour of the emission spectra, such as acridine [35], 7-methoxy-4-methyl-coumarins [36] systems. The band at the lower wavelength in the spectra, corresponds to the non-aggregated compounds and a peak at the higher wavelength is caused by the emission of aggregated and aromatic units. The investigated compound shows single emission band in most of the solvents. The shoulder found in the spectra of Acetone, DMF and CAN indicates the formation of two excited states in these solvents.

Table 1 Solvatochromic data of N-CAN

Solvents	$\lambda_a nm$	$\lambda mm$					
		, y	$\overline{v}_a(cm^{-1})$	$\overline{v}_f(cm^{-1})$	$\left(\overline{v}_a - \overline{v}_f\right)$ $(cm^{-1})$	$\frac{\frac{1}{2}\left(\overline{v}_{a}+\overline{v}_{f}\right)}{(cm^{-1})}$	$E_T^N$
Hexane	272.07	390.16	36755.25	25641.03	11114.22	31198.14	0.009
Toluene	284.02	405.46	35208.79	24663.35	10545.44	29936.07	0.099
CHCl <sub>3</sub>	276.07	402.00	36222.70	24875.62	11347.08	30549.16	0.254
EA	273.80	394.00	36523.01	25316.46	11206.55	30919.73	0.22
ACN	273.43	397.68	36572.43	25145.85	11432.50	30859.14	0.46
DCM	275.67	388.00	36275.26	25773.2	10502.06	31024.23	0.31
Dioxane	274.80	388.75	36349.10	25723.47	10625.62	31636.28	0.16
Acetone	274.30	400.00	36456.43	25000.00	11456.43	30728.22	0.35
DMF	275.89	409.00	36246.33	24449.88	11796.45	30348.10	0.39
EtOH	273.39	402.11	36577.78	24868.82	11708.97	30723.3	0.65
МеОН	274.44	391.94	36437.84	24937.66	11500.18	30687.75	0.76





**Fig. 4** The studies of variation of Stokes shift vs Various equation. **a**The variation of Stoke's shift with  $F_1(\varepsilon, \eta)$  using Lippert-Mataga equation for N-CAN, **b** The variation of Stoke's shift with  $F_2(\varepsilon, \eta)$  using Bakshiev's

The quinone molecule exhibits dual emission in aprotic solvents due to the presence of two close-lying excited states [37]. An emission band is observed due to the forbidden  $n \rightarrow \pi^*$  electronic transition which arises due to the interaction of the lone pair of nitrogen atoms with the solvent molecules. The emission band of the N-CAN compound was observed between 350 nm to 460 nm. As the solvent polarity was

 Table 2
 Statistical treatment of the correlation of solvent spectral studies of N-CAN

Compound	Method	Slope	Correlation	Data
N-CANs	Lippert Mataga	3260.80	0.9000	8
	Bakshiev's	1286.37	0.9200	8
	Chamma-Viallet	-2701.2	0.8998	7
	E <sup>N</sup> T	3378.90	0.8009	7

equation for N-CAN, **c** The variation of stoke's shift with  $F_3(\varepsilon, \eta)$  using Kawski-Chamma-Viallet equation for N-CAN **d** The variation of Stoke's shift with  $E^N_T$  for N-CAN

measured from Hexane to methanol, the emission maximum is shifted from shorter wavelength to longer wavelength. The bathochromic shift from 362 nm to 423 nm, corresponding to a 61 nm shift confirms a  $\pi \rightarrow \pi^*$  electronic transitions which are borne out from the conjugation between the Ketone and the aromatic ring system. On increasing the solvent polarity the stoke shift value increase from  $11,114.22 \text{ cm}^{-1}$  in hexane to  $11,500 \text{ cm}^{-1}$  in methanol. The magnitude of stokes shifts indicates the operation of partial intramolecular charge transfer from donor (Carbonyl) to acceptor (Amine). All these data imply that the molecule is influenced by parameters such as polarity, hydrogen bond donor-acceptor strength. In the study of the emission spectra of N-CAN compound, the non-polar solvents and the borderline aprotic solvents only exhibit a bathochromic shift. In the case of polar protic solvents and polar aprotic solvents such as acetone, DMF, IPA, ethanol, and methanol a hypsochromic shift due to the strong hydrogen bonding formation between the heteroatom present in the N-

Table 3	Ground state and Excited State dipole moments of N-CAN										
	$a^{o}_{(\mathrm{\AA})}$	$\mu_g^{\ a}{}_{(\mathrm{D})}$	$\mu_e^{\ b}(\mathbf{D})$	$\mu_g^{\ c}{}_{(\mathrm{D})}$	$\mu_e^{d}{}_{(\mathrm{D})}$	$\mu_e^{e}{}^{(\mathrm{D})}$	$\mu^{f}_{e(\mathrm{D})}$	$\mu_e^{g}{}_{(\mathrm{D})}$	$\mu_e^{h}{}^{(\mathrm{D})}$	$\frac{\mu_e}{\mu_g}$ i	$\Delta \mu^{j}$
N-CAN	4.19	0.51	4.76	1.77	4.78	4.76	6.65	4.77	6.21	2.70	2.73
Debye (E	() = 3.33564  x	$10^{-30}$ cm =	$10^{-18}$ esu cm								

Theoretical ground state dipole moment using DFT studies (B3LYP level)

<sup>b</sup> Theoretical excited state dipole moment using DFT studies (B3LYP level)

<sup>c</sup> The ground state dipole moment calculated using Eq. 10

<sup>d</sup> The excited dipole moment calculated using Eq. 11

<sup>e</sup> The excited dipole moment calculated using Eq. 12

<sup>f</sup> The change of excited dipole moment calculated from Lippert-Mataga expression

<sup>g</sup> The excited dipole moment calculated from Bakshiev's expression

<sup>h</sup> The excited dipole moment calculated from Kawaski-Chamma-Viallet expression

<sup>i</sup> The ratio of excited state and ground state value

<sup>j</sup> The change in dipole moment calculated from Reichardt expression

CAN compound was observed. Thus it reveals that the molecule is more stabilized in the excited state in polar solvents than the ground state implying that the expected excited state dipole moment should be higher.

# **Experimental and Theoretical Calculations of Dipole Moments**

Figure 3, the ground state geometry of the compound is fully optimized at the semi empirical AM1 level and refined at B3LYP level using a standard 6–31 (g) basis set on all atoms with the Gaussian 09 suite of the program. The N-CAN spectroscopic properties were investigated by solvatochromic behaviour using relevant solvent polarity scales of Lippert-Mataga correlation, Bakshiev's correlation and Kawski-Chamma-Viallet correlation methods. The stokes shift values are given in Table 1. The stokes shift value can be plotted against polarity functions  $F_1(\varepsilon, \eta)$ ,  $F_2(\varepsilon, \eta)$ ,  $F_3(\varepsilon, \eta)$  and  $E_T^N$ . The stokes shift value plotted against  $F_1(\varepsilon, \eta), F_2(\varepsilon, \eta)$  are given in Fig. 4a, b. The average values of stokes shift are plotted against  $F_3(\varepsilon, \eta)$  and  $E_T^N$  given in Fig. 4c, d. The stokes shift range was plotted against polarity function of the various solvents. The different solvents polarity function values of Lippert-Mataga, Bakshiev's, Kawaki-Chamma-Viallet are given in ESM (Electronic supplementary material). The linear progression was done and the data was fit to a straight line and the corresponding values of the slopes are given in Table 2. In most of the cases the correlation co-efficient are higher than 0.90 and it indicates a good linearity for Z1, Z2, Z3 with selected number of stokes shift data points. Generally, the deviation from linearity may be due to specific solute-solvent interactions. The dipole moment of N-CAN in the ground state and excited state changes due to electron densities. The invariance of absorption spectra and emission spectra with solvent polarity suggests that the excited state values are more sensitive than the ground state values. The dipole moment excited state value of Lippert-Mataga (6.65 D), Kawski-Chamma-Viallet (6.21 D) is higher than the value derived from the Bakshiev's method (4.77 D). The different dipole moment values clearly explain that the N-CAN compound has more charge transfer in the emitting state. The radius of the N-CAN was calculated using the Suppan Eq. (10). The dipole moments are assumed to be parallel and the ground state and excited state values are calculated using Eqs. (7) and (8). The angle between ground and excited dipole moments was calculated from Eq. (12). From Table 3, it is observed that the value of excited state dipole moment is more than the ground state dipole moment. Therefore we conclude that the excited state is more polar than the ground state. Assuming that excited state dipole moment is almost parallel with the ground state. The angle between ground state dipole moment (1.77 D) and excited state dipole moment (4.78 D) were calculated and the value was found to be 0.98°, which supports that the dipole moments are nearly parallel. N-CAN compound has higher values of dipole moment due to the intermolecular hydrogen bond formation ability.

# Conclusion

We have studied the photophysical properties of a quinone derivative. The study of solvent effects on the absorption and fluorescence spectra can be contributed to elucidate the internal structure of the organic compound and to estimate the electro-optical molecular parameters such as dipole moments or polarizabilities of the compound. In absorption spectra, we observed a red shift upon increasing the solvent polarity, which indicates the occurrence of a  $\pi \rightarrow \pi^*$  transition in the molecule. In the emission spectra, we observed both bathochromic shift and hypsochromic effect on increasing the solvent polarity. The experimental excited state dipole moment of N-CAN was estimated using Lippert-Mataga, Bakshiev's, Kawski-Chamma-Viallet and Reichardt correlation methods. The quinone derivative has a higher dipole moment in the excited state when compared to the ground state dipole moment, which indicates that the excited state dipole moment is more polar than the ground state dipole moment.

Acknowledgements The authors thank the Management and the authorities of Karunya University, Coimbatore, for their kind support, constant encouragement.

# Reference

- O'Malley PJ (2001) Electronic structure studies of Quinones and Semiquinones: accurate calculation of spin densities and electron paramagnetic resonance parameters. Antioxid Redox Signal 3(5):825–838
- Ma W, Long YT (2014) Quinone/hydroquinone-functionalized biointerfaces for biological applications from the macro- to nanoscale. Chem Soc Rev 43(1):30–41
- John OM, Vincent JD, Pugh D (1987) Non-linear optical properties of organic molecules. Part 2. Effect of conjugation length and molecular volume on the calculated hyperpolarisabilities of polyphenyls and polyenes. J Chem Soc Perkin Trans 2:1351–1355
- 4. Lakowicz JR (2006) Principles of fluorescence spectroscopy, third edn. KLuwer Academic/ Plenum Press, New York
- Ooshika Y (1954) Absorption spectra of dyes in solution. J Phys Soc Jpn 9:594–602
- Mataga N (1963) Solvent effects on the absorption and fluorescence spectra of naphthylamines and isomeric aminobenzoic acids. Bull Chem Soc Jpn 36:654–659
- Czekella J (1960) Electrical fluorescence polarization: the determination of dipole moments of excited molecule from the polarization degree of fluorescence in strong electric field, Z. Elektrochem 64:1221
- 8. Czekella J (1961) Two electro-optical methods to determine dipole moments of excited molecules. Chimica 15:26
- Hass MP, Warman JM (1982) Photon induced molecular change separation studied by nanosecond time-resolved microwave conductivity. Chem Phys 73:35
- Lombardi JR (1998) Solvatochromic shifts: a reconsideration. J Phy Chem A 102:2817
- Liptay W, Lim EC (1961) Excited states, vol.1, academic Press, New York, 1974. J Czekella Zeitschrift fur Chimica 15:26–29
- Mataga N, Kaifu Y, Koizumi M (1956) Solvent effects upon fluorescence spectra and the dipolemoment of the excited molecule. Bull Chem Soc Jpn 29:465–470
- 13. Bakshiev's NG (1964) Universal intermolecular interactions and their effect on the position of the electronic spectra of molecules in two-component solutions. Opt Spektrosk 16:821
- Bilot L, Kawski A (1962) To theory of the influence of solvents on the electron spectra of molecules. Zeitschrift f
  ür Naturforschung A 17:621–627
- Chamma A, Viallet P (1970) Determination of the dipole moment of a molecule in an excited singlet state: application to indole, benzimidazole and the indazole. Acad Sci Paris Ser 270 C:1901
- Reichardt C (1994) Solvatochromic dyes as solvent polarity indicators. Chem Rev 94:2319
- Giri R (1992) M.M. Bajaj, estimation of excited state dipole moment of substituted coumarins. Curr Sci 62:522–525

- Sharma N, Sapan K, Rastogi RC (2007) Solvatochromic study of excited state dipole moments of some biologically active indoles and tryptamines. Spectrochim Acta Part A 66:171–176
- Aaron JJ, Gaye MD, Parkanyi C, Cho NS, Szentpaly LV (1987) Experimental and theoretical dipole moments of purines in their ground and lowest excited singlet states. J Mol Struct 156:119–135
- Inamdar SR, Nadaf YF, Mulimani BG (2004) Ground and excited state dipole moments of some exalite UV laser dyes from solvatochromic method using solvent polarity parameters. J Mol Struct (THEOCHEM) 678:177–181
- Aaron JJ, Times A, Gaye MD, Parkanyi C, Boniface C, Bieze TW (1991) Effects of solvent on the electronic absorption and fluorescence spectra of quinazolines, and determination of their ground and excited singlet-state dipole moments. Spectrochim Acta A 47: 419–424
- Aaron JJ, Maafi M, Párkányi C, Boniface C (1995) Quantitative treatment of the solvent effects on the electronic absorption and fluorescence spectra of acridines and phenazines. The ground and first excited singlet-state dipole moments. Spectrochim Acta A 51: 603–615
- Sasirekha V, Umadevi M, Ramakrishnan V (2008) Solvatochromic study of 1,2-dihydroxyanthraquinone in neat and binary solvent mixtures. Spectrochim Acta A 69:148–155
- Acemioglu B, Arık M, Efeoglu H, Onganer Y (2001) Solvent effect on the ground and excited state dipole moments of fluorescein. J Mol Struct (THEOCHEM) 548:165–171
- Kumar S, Jain SK, Rastogi RC (2001) An experimental and theoretical study of excited-state dipole moments of some flavones using an efficient solvatochromic method based on the solvent polarity parameter, ENT. Spectrochim Acta A 57:291–298
- Lyman R et al (1974) Dipole moments of some 3-and 4-substituted phthalimides and phthalic anhydrides. Influence of steric and resonance effects. J Organomet Chem 39(11):1527–1531
- Geethanjali HS, Nagaraja D, Melavanki RM (2015) Estimation of dipole moments and quantum yield of 5-chloro-2-methoxyphenyl Boronic acid in different solvents environment. J Fluoresc 25(3): 745–753
- Almeida KJ et al (2001) A Monte Carlo–quantum mechanical study of the solvatochromism of pyrimidine in water and in carbon tetrachloride. Phys Chem Chem Phys 3:1583–1587
- Suppan P (1983) Excited-state dipole moments from absorption/ fluorescence solvatochromic ratios. Chem Phys Lett 94:272
- Reichardt C, Welton T (2011) Solvents and solvent effects in organic chemistry, 4th edn. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim
- Reichardt C (1992) Solvatochromism, thermochromism, piezochromism, halochromism, and chiro-solvatochromism of pyridinium N-phenoxide betaine dyes. Chem Soc Rev 21:147–153
- Ravi M, Samanta A, Radhakrishnan TP (1994) Excited state dipole moments from an efficient analysis of solvatochromic stokes shift data. J Phys Chem 98(37):9133–9136
- Ravi M, Samanta A, Radhakrishnan TP (1995) Excited-state dipole moments of some hydroxycoumarin dyes using an efficient solvatochromic method based on the solvent polarity parameter, ETN. J Chem Soc Faraday Trans 91:2739–2742
- 34. Rabek JF, Scott GW (1989) Photochemistry and photophysics. CRC Press, Boca Raton
- Kellmann A (1977) Intersystem crossing and internal conversion quantum yields of acridine in polar and nonpolar solvents. J Phys Chem 81:1195–1198
- Uchiyama S, Takehira K, Yoshihara T, Tobita S, Ohwada T (2006) Environment- sensitive fluorophore emitting in protic environments. Org Lett 8:5869–5872
- Haidekker MA, Theodorakis EA (2016) Ratiometric mechanosensitive fluorescent dyes: design and applications. J Mater Chem C 4:2707–2718